Hole Pairs in the Two-Dimensional Hubbard Model

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The interactions between holes in the Hubbard model, in the low density, intermediate to strong coupling limit, are investigated. Dressed spin polarons in neighboring sites have an increased kinetic energy and an enhanced hopping rate. Both effects are of the order of the hopping integral and lead to an effective attraction at intermediate couplings. Our results are derived by systematically improving mean field calculations. The method can also be used to derive known properties of isolated spin polarons.

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The nature of the low energy excitations in the Hubbard model has attracted a great deal of attention. Close to half filling, a large amount of work suggests the existence of spin polarons, made of dressed holes, which propagate within a given sublattice with kinetic energy of the order of $J = \frac{4t^2}{U}$ [1,2], where t is the hopping integral and U the on site Coulomb repulsion. These results are consistent with similar calculations in the strong coupling, low doping limit of the Hubbard model, the $t-J$ model [3–5]. There is also evidence for an effective attraction between these spin polarons [6–10].

In the present work, we analyze the dynamics of spin polarons and the interactions between them by means of a systematic expansion around mean field calculations of the Hubbard model on the bipartite square lattice. Two spin polarons in neighboring sites experience an increase in their internal kinetic energy, due to the overlap of the charge cloud. This repulsion is of the order of t. In addition, a polaron reduces the obstacles for the diffussion of another, leading to an assisted hopping term which is also of the order of t. The combination of these effects is an attractive interaction at intermediate values of U/t.

Use of the Unrestricted Hartree Fock (UHF) approximation in finite clusters provides a first order approximation to the spin polaron near half filling. As discussed elsewhere, this approximation describes well the undoped, insulating state at half filling [11]. A realistic picture of the spin wave excitations is obtained by adding harmonic fluctuations by means of the time dependent Hartree Fock approximation (RPA) [12]. At intermediate and large values of U/t, the most stable HF solution with a single hole is a spin polaron [11]. This solution is replaced by a fully ferromagnetic one at sufficiently large values of U/t [13]. Approximately half of the charge of the hole is located at a given site in the spin polaron solution. The spin at that site is small and it is reversed with respect to the antiferromagnetic background. The remaining charge is concentrated in the four neighboring sites. A number of alternative derivations lead to a similar picture of this small spin bag [14–17]. A similar solution is expected to exist in the $t-J$ model.

As usual in mean field theories, the spin polaron solution described above breaks symmetries which must be restored by quantum fluctuations. In particular, it breaks spin symmetry and translational invariance. Spin isotropy must exist in finite clusters. However, it is spontaneously broken in the thermodynamic limit, due to the presence of the antiferromagnetic background. Hence, we do not expect that the lack of spin invariance is a serious drawback of the Hartree Fock solutions. In any case, spin isotropy can be restored, starting from the mean field wavefunction, by projecting out the components which do not have a predetermined spin. Results obtained for small clusters [18,19] show a slight improvement of the energy, which goes to zero as the cluster size is increased. On the other hand, translational invariance is expected to be present in the exact solution of clusters of any size. Thus, we have improved the mean field results by hybridizing a given spin polaron solution with all wavefunctions obtained from it by lattice translations. This procedure is equivalent to the configuration interaction (CI) method used in quantum chemistry. If the initial mean field solution is considered as the "classical" zeroth order approximation to the exact solution, this scheme can be described as the inclusion of instanton effects, in which the spin polarons tunnel between equivalent configurations. Finally, in addition to the previous corrections, we can add the zero point fluctuations around the RPA ground state [12]. This calculation does not change appreciably the results, although it is necessary to describe correctly the long ranged magnon cloud around the spin polaron [20].

A schematic picture of the initial one hole and two holes Hartree Fock wavefunctions used in this work is shown in Fig. 1. They represent the solutions observed at large values of U/t for the isolated polaron and two spin polarons on neighboring sites. Actually, charge localization is associated to the existence of bound states

which split from the top of the lower Hubbard band.

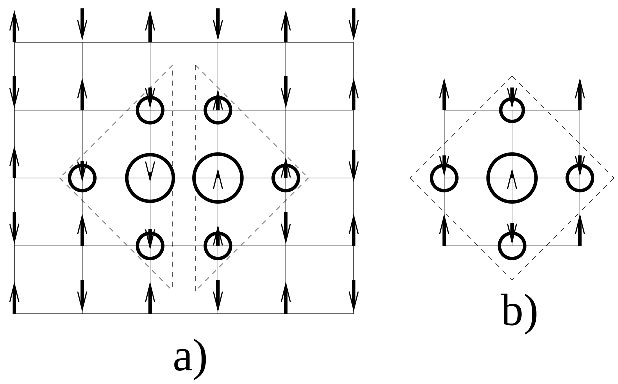

FIG. 1. a) Sketch of one of the bipolaron solutions, at large values of U/t, considered in the text. Circles denote the local charge, measured from half filling, and arrows denote the spins. There are two localized states marked by the dashed line. For comparison, the single polaron solution is shown in b).

Spin polaron wavefunctions localized at different sites are not orthogonal. Both wavefunctions overlap and non–diagonal matrix elements of the Hamiltonian need to be taken into account when mixing between configurations is considered. The procedure has been described in detail in [18], along with the energy improvements (with respect to UHF) introduced by this CI scheme. Calculations have been carried out on $L\times L$ clusters with periodic boundary conditions ($L \leq 12$) and $U \geq 8t$ [21]. Although larger clusters can be easily reached, no improvement of the results is achieved due to the short–range character of the interactions. The calculated dispersion of a single polaron is shown in Fig. 2. Because of the antiferromagnetic background, the band has twice the lattice periodicity. Exact calculations in finite clusters do not show this periodicity, as the solutions have a well defined spin and mix different background textures. As cluster sizes are increased, however, exact solutions tend to show the extra periodicity of our results. We interpret it as a manifestation that spin invariance is broken in the thermodynamic limit, because of the antiferromagnetic background. Hence, the lack of this symmetry in our calculations should not induce spurious effects. The only overlaps and matrix elements which are not negligible are those between polaron wavefunctions located in the same sublattice. Fig. 2 shows the polaron bandwidth as a function of U. It behaves as t^2/U (the fitted law is given in the caption of Fig. 2). Our scheme allows a straightforward explanation of this scaling. Without reversing the spin of the whole background, the polaron can only hop within a given sublattice. This implies an intermediate virtual hop into a site with an almost fully localized electron of the opposite spin. The amplitude of finding a reversed spin in this new site decays as t^2/U at large U. We find that the polaron band can be very well fitted by the expression: $\epsilon_k = \epsilon_0 + 4t_{11}\cos(k_x)\cos(k_y) + 2t_{20}[\cos(2k_x) + \cos(2k_y)] + 4t_{22}\cos(2k_x)\cos(2k_y) + 4t_{31}[\cos(3k_x)\cos(k_y) + \cos(k_x)\cos(3k_y)]$. For $U = 8t$, we get $t_{11} = 0.1899t$, $t_{20} = 0.0873t$, $t_{22} = -0.0136t$, and $t_{31} = -0.0087t$. All hopping integrals vanish as t^2/U in the large U limit for the reason given above. Also the energy gain with respect to UHF [18] behaves in this way. Let us mention, that all the features reported here are in good agreement with known results [1–4] for both the Hubbard and the $t-J$ models.

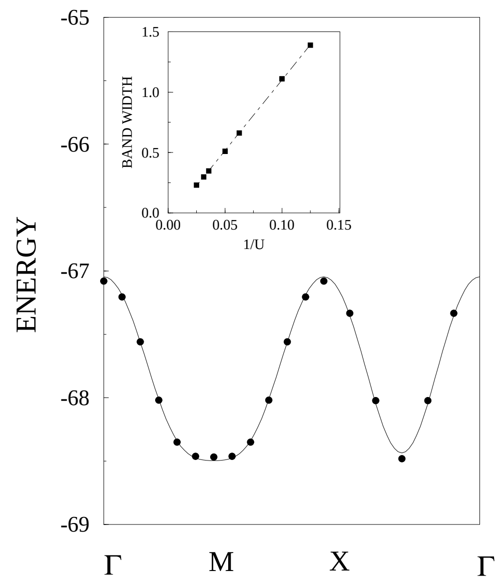

FIG. 2. Quasiparticle band structure for a single hole on 12×12 clusters of the square lattice with periodic boundary conditions and $U = 8t$ (filled circles). The continuous line corresponds to the fitted dispersion relation (see text). The inset shows the bandwidth as a function of t^2/U; the fitted straight line is $-0.022t + 11.11t^2/U$.

We now consider solutions with two spin polarons. The relevant UHF solutions are those with $S_z = 0$. In order to get some coupling, the centers of the two spin polarons must be located in different sublattices. The mean field energy increases as the two polarons are brought closer, although, for intermediate and large values of U, a locally stable Hartree Fock solution can be found with two polarons at arbitrary distances. We have not attempted to do a full CI analysis of all possible combinations of two holes in a finite cluster. Instead, we have chosen a given mean field solution and hybridized it with all others obtained by a lattice translation or rotation. Clusters of sizes up to 10×10 were studied which, as in the case of the polaron, are large enough due to the short–range interactions between different configurations. The basis used for the two polarons at the shortest distance is shown in Fig. 3. This procedure leads to a set of bands for the two hole configurations. The number of bands is two or four, depending on the number of different config-

urations which can be obtained by rotations at a given site. Like in the single polaron case, we obtain a gain in energy, due to the delocalization of the pair.

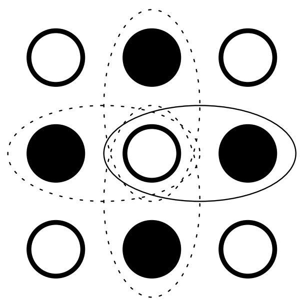

FIG. 3. Sketch of the bipolaron UHF wavefunctions used in this work. Note that the four wavefunctions are obtained by successive rotations of $\pi/2$. The complete basis set is produced by translation of these wavefunctions through the whole cluster.

The hole-hole interaction, i.e., the difference between the energy of a state built up by all configurations with the two holes at the shortest distance (separated by a vector of the set {1,0}) and the energy of the state having the holes at the largest distance possible at a given cluster is depicted in Fig. 4. Two holes bind for intermediate values of U [23]. This happens because the delocalization energy tends to be higher than the repulsive contribution obtained within mean field. The local character of the interactions is illustrated by the almost null dependence of the results shown in Fig. 4 on the cluster size. The energy gain of the two holes (with respect to UHF) in the two limiting configurations (at the shortest or largest distance possible) is given in the inset of Fig. 4. Note that, whereas in the case of the holes at the largest distance, the gain goes to zero in the large U limit, as for the isolated polaron, when the holes are separated by a $\{1,0\}$ vector the gain goes to a finite value. This result is not surprising, as the arguments given below suggest, and is in line with the results for the width of the quasiparticle band. The numerical results for L=6, 8 and 10 and U in the range $8t-5000t$ can be fitted by the following straight lines, $3.965t+14.47t^2/U$ (holes at the shortest distance) and $-0.007t+10.1t^2/U$ (holes at the largest distance). Thus, total bandwidth of the two bands obtained for holes in neighboring sites does not vanish in the infinite U limit (as the energy gain reported in Fig. 4). The internal consistency of our calculations is shown comparing the large U behavior of the two holes at the largest distance possible with the corresponding results obtained for the isolated polaron (compare this fitting with that given in the captions of Fig. 2) .

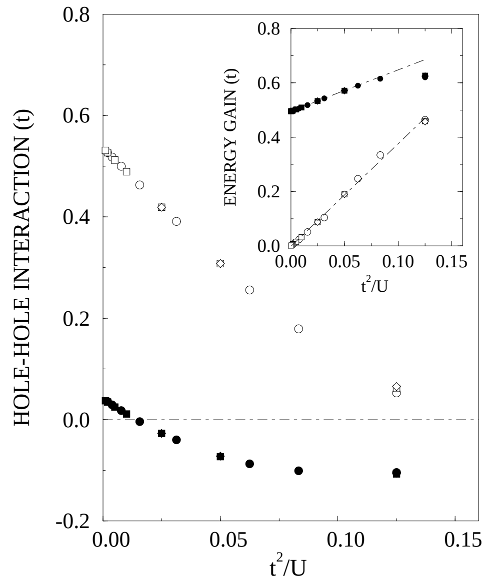

FIG. 4. Comparison of the hole-hole interaction (see main text for the definition) obtained within UHF (empty symbols) and CI (filled symbols) approximations. Results correspond to 6×6, (circles) 8×8 (squares) and 10×10 (diamonds) clusters with periodic boundary conditions. The inset shows the energy gain due to the inclusion of correlation effects via CI for both the configuration of holes located in neighboring positions (filled simbols) and holes that are maximally separated in the finite size cluster (empty simbols). The fitted straight lines are: $0.495t+1.53t^2/U$ (filled symbols) and $-0.002t+3.78t^2/U$ (empty symbols).

Both the behavior of the quasiparticle bandwidth and that of the energy gain with respect to UHF of the two holes at the shortest distance can be understood from arguments similar to those used for the single polaron. The hopping terms that are proportional to t at large U describe the rotation of a pair around the position of one of the two holes. Each hole is spread between four sites. In order for a rotation to take place, one hole has to jump from one of these sites into one of the rotated positions. This process can always take place without a hole moving into a almost fully polarized site with the wrong spin. In the single polaron case, as discussed before, the motion of a hole involves the inversion of, at least, one almost fully spin polarized site, in the large U limit. As a consequence, the delocalization of polaron pairs on neighboring sites leads to a finite gain in energy, even as $U\to\infty$, as opposed to the single polaron case [18] or polaron pairs at the largest distance (see inset of Fig. 4).

The possibility of hole assisted hopping was discussed in [24], in a different context. It always leads to superconductivity. In our case, we find a contribution, in the large U limit, of the type:

$$\mathcal{H}_{hop}=\sum\Delta t c^{\dagger}{}_{i,j;s}c_{i,j;s}(c^{\dagger}{}_{i+1,j;\bar{s}}c_{i,j+1;\bar{s}}+ \\ + c^{\dagger}{}_{i-1,j;\bar{s}}c_{i+1,j;\bar{s}}+h.c.+\text{perm}) \quad (1)$$

This term admits the BCS decoupling $\Delta t \langle c^\dagger_{i,j;s} c^\dagger_{i+1,j;\bar{s}} \rangle c_{i,j;s} c_{i,j+1;\bar{s}} + h.c. + ...$ It favors superconductivity with either s or d wave symmetry, depending on the sign of Δt. Since we find $\Delta t > 0$, d wave symmetry follows.

An interesting question is whether the holes would tend to segregate when more holes are added to the cluster. In order to investigate this question, we have calculated the total energies for four holes centered on a square and two separated bipolarons with holes at the shortest distance. Two (four) configurations (plus translations) were included in each case. The results for 4 holes on a 8×8 cluster and $U = 8t$ are, $-34.06t$ (four holes on a square) and $-34.48t$ (two bipolarons). Note that although the fourfold–polaron has also hopping terms which do not vanish in the infinite U limit, they are weaker than in the bipolaron case. These results indicate that for large and intermediate U no hole segregation takes place (for small U see below) and that the most likely configuration is that of separated bipolarons.

The picture presented above is consistent with other analytical and numerical studies of hole-hole pairing in real space [25,22,26,27] at low fillings and intermediate to large values of U/t. As U is reduced, the size of the spin polarons increases and becomes elongated along the diagonals of the square lattice. The most likely solutions of the Hartree-Fock calculations are domain walls which separate antiferromagnetic regions [28–30,11]. The breakdown of translational symmetry associated with these solutions is probably real and not just an artifact of the Hartree Fock solution, as in the case discussed previously. Hence, we expect a sharp transition between a regime of small spin polarons with an effective attraction and striped phases at low U. Note, however, that the scheme presented here, based on mean field solutions plus corrections, is equally valid in both cases.

Summarising, we have analyzed the dynamics of spin polarons and their interactions by systematically improving the mean field approximation to the Hubbard model. Our scheme gives an intutive framework in which the appearance of attraction between holes can be understood.

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